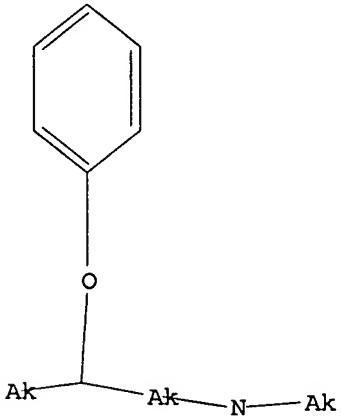
```
=> d his

     (FILE 'HOME' ENTERED AT 09:19:10 ON 29 AUG 2007)

     FILE 'REGISTRY' ENTERED AT 09:19:16 ON 29 AUG 2007
L1             STRUCTURE UPLOADED
L2             SCREEN 1135
L3             SCREEN 1146
L4             SCREEN 95
L5           6 S (L1 AND (L2 AND L3 AND L4)) SAM
L6        2513 S (L1 AND (L2 AND L3 AND L4)) SSS FULL
               SAV TEM L6 BRD597835/A

     FILE 'CAPLUS' ENTERED AT 09:20:21 ON 29 AUG 2007
L7         643 S L6

     FILE 'REGISTRY' ENTERED AT 09:20:27 ON 29 AUG 2007

     FILE 'STNGUIDE' ENTERED AT 09:20:30 ON 29 AUG 2007

     FILE 'REGISTRY' ENTERED AT 09:25:08 ON 29 AUG 2007
L8             STRUCTURE UPLOADED
L9          50 S L8 SAM SUB=L6
L10       1097 S L8 SSS FULL SUB=L6

     FILE 'CAPLUS' ENTERED AT 09:26:22 ON 29 AUG 2007
L11        311 S L10

     FILE 'STNGUIDE' ENTERED AT 09:26:31 ON 29 AUG 2007

     FILE 'REGISTRY' ENTERED AT 09:28:07 ON 29 AUG 2007
L12            STRUCTURE UPLOADED
L13         50 S L12 SAM SUB=L6

     FILE 'STNGUIDE' ENTERED AT 09:28:46 ON 29 AUG 2007

     FILE 'REGISTRY' ENTERED AT 09:38:59 ON 29 AUG 2007
L14       1069 S L12 SSS FULL SUB=L6
               SAV TEM ELE597835/A L14

     FILE 'CAPLUS' ENTERED AT 09:39:23 ON 29 AUG 2007
L15        294 S L14
L16          1 S US2006-597835/APPS
L17          1 S L15 AND L16

     FILE 'STNGUIDE' ENTERED AT 09:39:56 ON 29 AUG 2007

     FILE 'REGISTRY' ENTERED AT 09:42:11 ON 29 AUG 2007
L18            STRUCTURE UPLOADED
L19          5 S L18 SAM SUB=L6
L20        182 S L18 SSS FULL SUB=L6

     FILE 'CAPLUS' ENTERED AT 09:42:43 ON 29 AUG 2007
L21         23 S L20
L22          1 S L16 AND L21
L23          0 S L16 NOT L21
L24         22 S L21 NOT L16

     FILE 'REGISTRY' ENTERED AT 09:43:31 ON 29 AUG 2007

=> d l1
L1 HAS NO ANSWERS
L1             STR
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

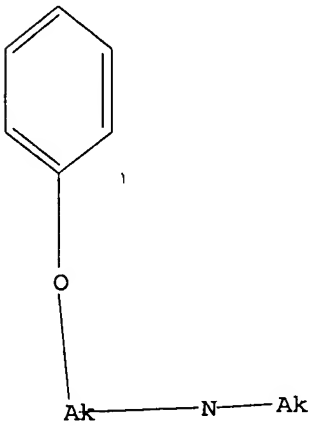
Structure attributes must be viewed using STN Express query preparation.

=> d l8
L8 HAS NO ANSWERS
L8 STR



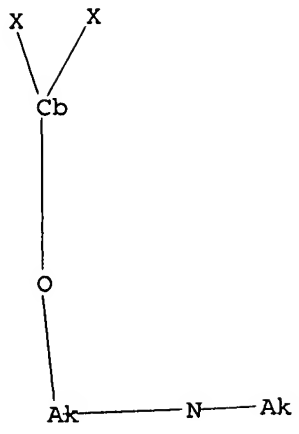
Structure attributes must be viewed using STN Express query preparation.

=> d l12
L12 HAS NO ANSWERS
L12 STR



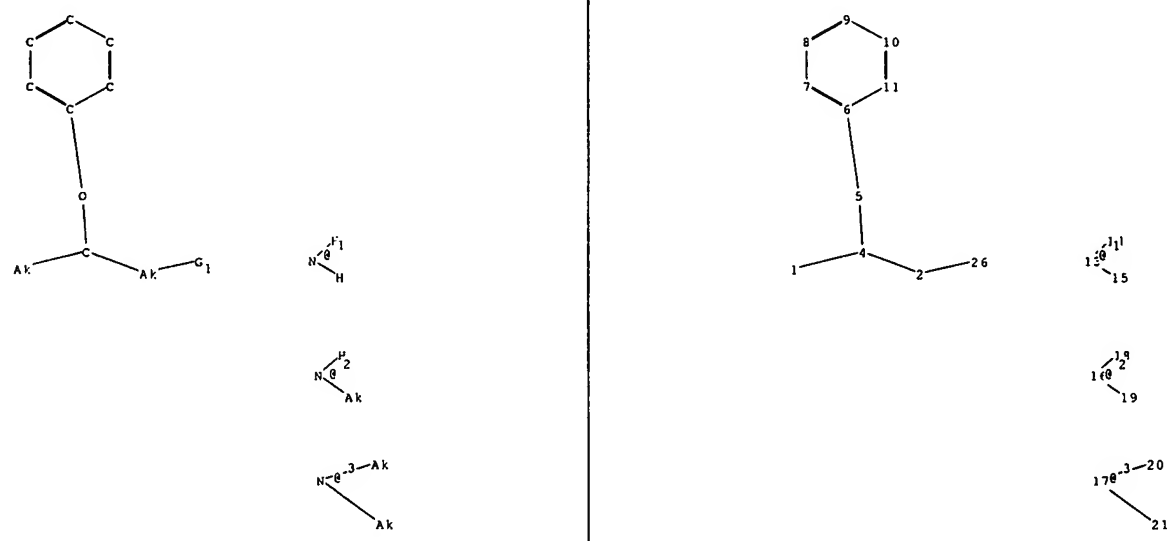
Structure attributes must be viewed using STN Express query preparation.

=> d l18
L18 HAS NO ANSWERS
L18 STR



Structure attributes must be viewed using STN Express query preparation.

C:\Program Files\Stnexp\Queries\10597835-brd.str

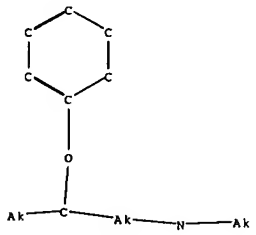


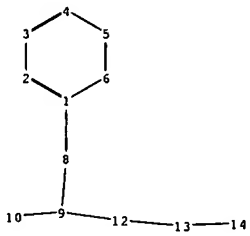
chain nodes :
1 2 4 5 13 14 15 16 17 18 19 20 21 26
ring nodes :
6 7 8 9 10 11
chain bonds :
1-4 2-4 2-26 4-5 5-6 13-14 13-15 16-18 16-19 17-20 17-21
ring bonds :
6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-4 2-4 2-26 4-5 5-6 13-14 13-15 16-18 16-19 17-20 17-21
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11
isolated ring systems :
containing 6 :

G1:[*1],[*2],[*3]

Connectivity :
2:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS
26:CLASS

C:\Program Files\Stnexp\Queries\10597835-elected.str

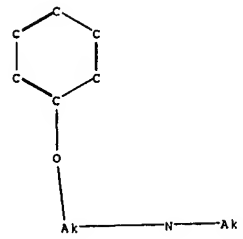


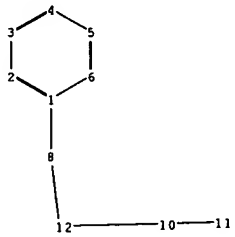


chain nodes :
8 9 10 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
1-8 8-9 9-10 9-12 12-13 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-8 8-9 9-10 9-12 12-13 13-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
10:1 E exact RC ring/chain 12:2 E exact RC ring/chain 14:1 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 12:CLASS
13:CLASS 14:CLASS

C:\Program Files\Stnexp\Queries\10597835-elected-narrow.str

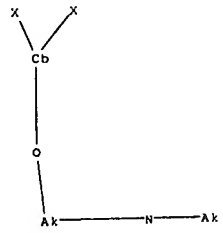


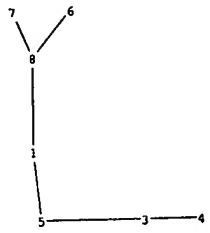


chain nodes :
8 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
1-8 8-12 10-11 10-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-8 8-12 10-11 10-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Connectivity :
11:1 E exact RC ring/chain 12:2 E exact RC ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 10:CLASS 11:CLASS 12:CLASS

C:\Program Files\Stnexp\Queries\597835-elect-narrow-2.str



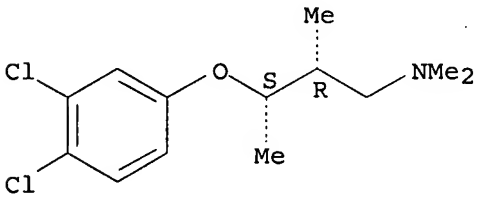


chain nodes :
1 3 4 5 6 7 8
chain bonds :
1-5 1-8 3-4 3-5 6-8 7-8
exact/norm bonds :
1-5 1-8 3-4 3-5 6-8 7-8

Connectivity :
4:1 E exact RC ring/chain 5:2 E exact RC ring/chain
Match level :
1:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom

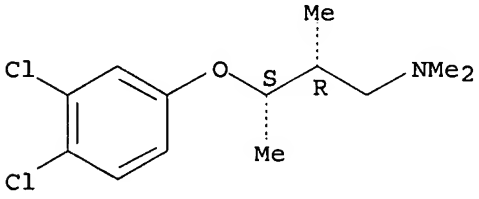
L24 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:934783 CAPLUS
DN 145:488808
TI Expanding the medicinal chemistry toolbox: stereospecific generation of methyl group-containing propylene linkers
AU Bosse, Kristopher; Marineau, Jason; Nason, Deane M.; Fliri, Anton J.; Segelstein, Barb E.; Desai, Kishor; Volkmann, Robert A.
CS Pfizer Global Research and Development, Groton Laboratories, Pfizer Inc., Groton, CT, 06340, USA
SO Tetrahedron Letters (2006), 47(41), 7285-7287
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Ltd.
DT Journal
LA English
OS CASREACT 145:488808
AB Use of alkyl substituted propylene linkers as a strategy for fine-tuning the biol. activity of medicinal agents requires ready access to these substrates. Herein, a general strategy is described for stereospecifically generating 18 chiral mono- and di-methylpropylene linkers. All twelve vicinal 1,2-propylene targets were generated from methyl-3-hydroxybutanoate and all 1,3-disubstituted targets from pentane-2,4-diol.
IT 914461-73-7P 914461-88-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereospecific generation of (aryloxy)alkylamines containing chiral Me group-containing propylene linkers)
RN 914461-73-7 CAPLUS
CN 1-Butanamine, 3-(3,4-dichlorophenoxy)-N,N,2-trimethyl-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 914461-88-4 CAPLUS
CN 1-Butanamine, 3-(3,4-dichlorophenoxy)-N,N,2-trimethyl-, hydrochloride, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



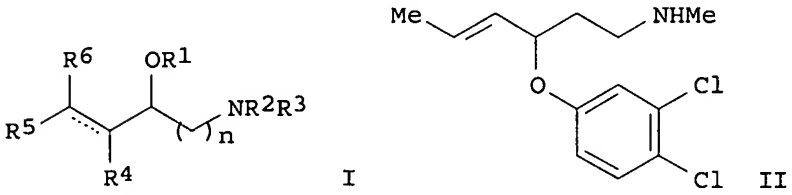
● HCl

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:193925 CAPLUS
DN 144:253896
TI Preparation of substituted aryloxy alkylamines as monoamine neurotransmitter re-uptake inhibitors
IN Eriksen, Birgitte L.; Peters, Dan; Nielsen, Elsebet Oestergaard; Scheel-Krueger, Joergen; Olsen, Gunnar M.
PA Neurosearch A/S, Den.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2006021564	A1	20060302	WO 2005-EP54151	20050824
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
EP 1784381	A1	20070516	EP 2005-774064	20050824
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRAI DK 2004-1290	A	20040826		
US 2004-605175P	P	20040830		
WO 2005-EP54151	W	20050824		

OS CASREACT 144:253896; MARPAT 144:253896
GI

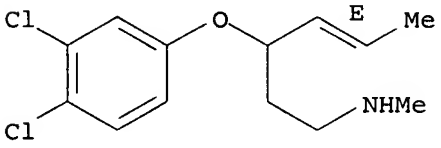


AB Title compds. I (R1 = aryl, optionally substituted with halo, CF3, CF3O, cyano, OH, NH2, NO2, alkoxy, cycloalkoxy, alkyl, cycloalkyl, alkenyl, alkynyl with the proviso that R1 ≠ 2,5-disubstituted Ph or 2,4,5-trisubstituted Ph; n = 1, 2; R2, R3 = H, alkyl, single or double bond; R4, R5 = H, alkyl; R4R5 together with the carbon atoms to which they are attached form a three-membered carbocyclic ring; R6 = H, alkyl), their isomers, or pharmaceutically acceptable salts, were prepared for the treatment of pain, nervous system disorders, etc. (no data). For example, title compound II was prepared from the coupling reaction of (E)-1-methylamino-hex-4-en-3-ol with 3,4-dichlorofluorobenzene, followed by the addition of fumaric acid to isolate II as its fumarate salt.
IT 877475-10-0P 877475-11-1P 877475-12-2P
877475-13-3P 877475-14-4P 877475-15-5P
877475-16-6P 877475-17-7P 877475-22-4P

877475-23-5P 877475-24-6P 877475-25-7P
877475-26-8P 877475-27-9P 877475-28-0P
877475-29-1P 877475-30-4P 877475-31-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted aryloxy alkylamines as monoamine neurotransmitter re-uptake inhibitors)

RN 877475-10-0 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N-methyl-, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

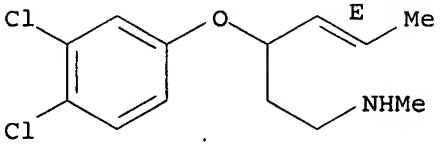


RN 877475-11-1 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N-methyl-, (4E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-10-0
CMF C13 H17 Cl2 N O

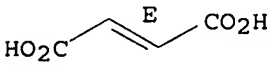
Double bond geometry as shown.



CM 2

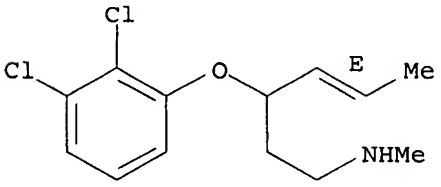
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 877475-12-2 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-dichlorophenoxy)-N-methyl-, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

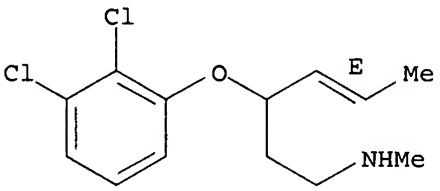


RN 877475-13-3 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-dichlorophenoxy)-N-methyl-, (4E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-12-2
CMF C13 H17 Cl2 N O

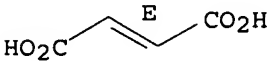
Double bond geometry as shown.



CM 2

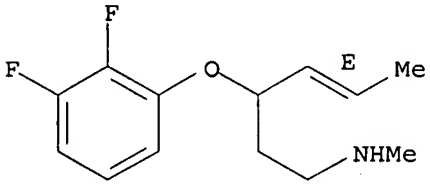
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 877475-14-4 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-difluorophenoxy)-N-methyl-, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

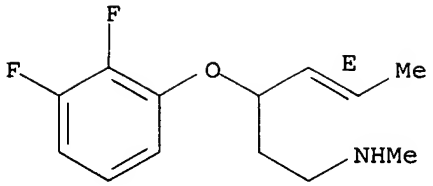


RN 877475-15-5 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-difluorophenoxy)-N-methyl-, (4E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-14-4
CMF C13 H17 F2 N O

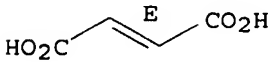
Double bond geometry as shown.



CM 2

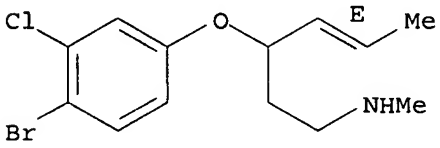
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 877475-16-6 CAPLUS
CN 4-Hexen-1-amine, 3-(4-bromo-3-chlorophenoxy)-N-methyl-, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

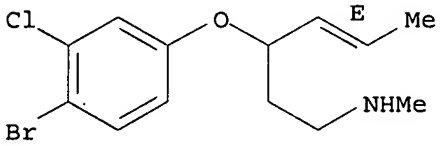


RN 877475-17-7 CAPLUS
CN 4-Hexen-1-amine, 3-(4-bromo-3-chlorophenoxy)-N-methyl-, (4E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-16-6
CMF C13 H17 Br Cl N O

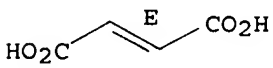
Double bond geometry as shown.



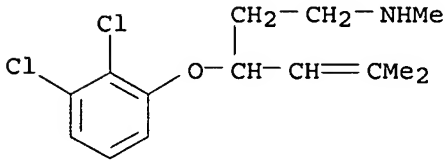
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



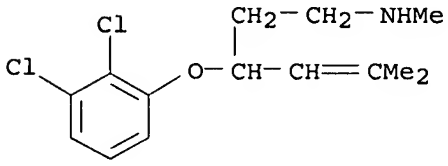
RN 877475-22-4 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-dichlorophenoxy)-N,5-dimethyl- (9CI) (CA INDEX NAME)



RN 877475-23-5 CAPLUS
CN 4-Hexen-1-amine, 3-(2,3-dichlorophenoxy)-N,5-dimethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

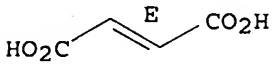
CRN 877475-22-4
CMF C14 H19 Cl2 N O



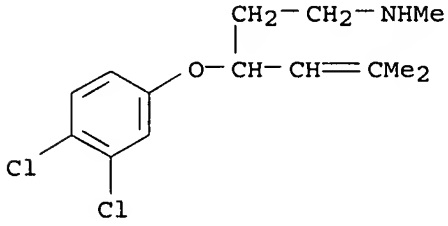
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



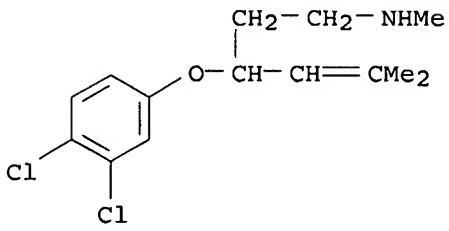
RN 877475-24-6 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N,5-dimethyl- (9CI) (CA INDEX NAME)



RN 877475-25-7 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N,5-dimethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

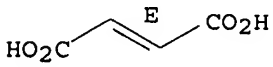
CRN 877475-24-6
CMF C14 H19 Cl2 N O



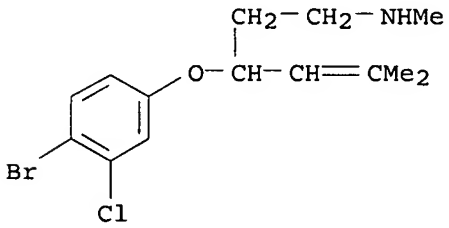
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



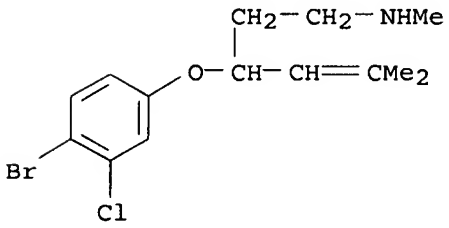
RN 877475-26-8 CAPLUS
CN 4-Hexen-1-amine, 3-(4-bromo-3-chlorophenoxy)-N,5-dimethyl- (9CI) (CA INDEX NAME)



RN 877475-27-9 CAPLUS
CN 4-Hexen-1-amine, 3-(4-bromo-3-chlorophenoxy)-N,5-dimethyl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

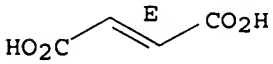
CRN 877475-26-8
CMF C14 H19 Br Cl N O



CM 2

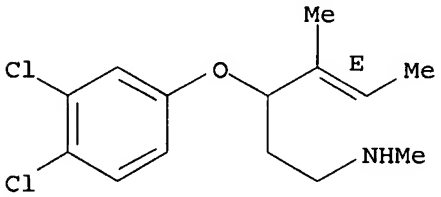
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 877475-28-0 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N,4-dimethyl-, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

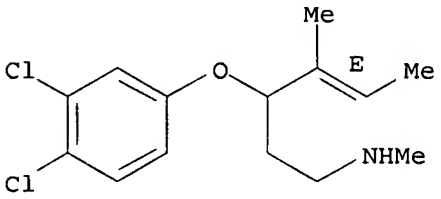


RN 877475-29-1 CAPLUS
CN 4-Hexen-1-amine, 3-(3,4-dichlorophenoxy)-N,4-dimethyl-, (4E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-28-0
CMF C14 H19 Cl2 N O

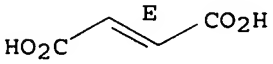
Double bond geometry as shown.



CM 2

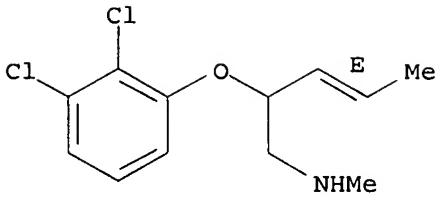
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 877475-30-4 CAPLUS
CN 3-Penten-1-amine, 2-(2,3-dichlorophenoxy)-N-methyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

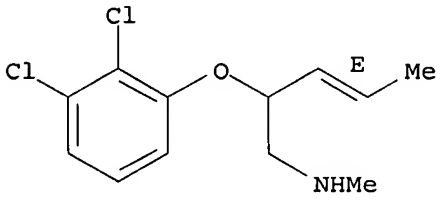


RN 877475-31-5 CAPLUS
CN 3-Penten-1-amine, 2-(2,3-dichlorophenoxy)-N-methyl-, (3E)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 877475-30-4
CMF C12 H15 Cl2 N O

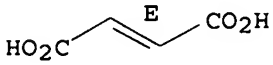
Double bond geometry as shown.



CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:636032 CAPLUS
DN 135:210829
TI Preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase
IN Cheshire, David; Connolly, Stephen; Cox, David; Mete, Antonio
PA Astrazeneca AB, Swed.
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001062714	A1	20010830	WO 2001-SE372	20010220

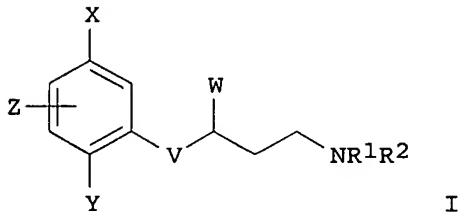
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,

YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	EP 1263715	A1	20021211	EP 2001-906491	20010220
	EP 1263715	B1	20040428		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003523993	T	20030812	JP 2001-561724	20010220
	AT 265423	T	20040515	AT 2001-906491	20010220
	US 2003065174	A1	20030403	US 2002-204845	20020822
	US 6900243	B2	20050531		
PRAI	GB 2000-4152	A	20000223		
	WO 2001-SE372	W	20010220		

OS MARPAT 135:210829

GI



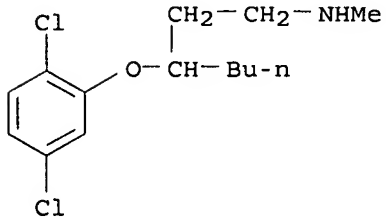
I

AB The title compds. [I; X, Y = alkyl, alkoxy, halo, etc.; Z = H, F; V = O, SOn, NR3; W = alkyl, alkenyl, alkynyl, etc.; R1, R2 = H, alkyl, cycloalkyl, etc.; or NR1R2 = (un)substituted 4-8 membered saturated azacyclic ring optionally incorporating one further heteroatom selected from O, S or NR6; R3 = H, alkyl; R6 = H, (un)substituted alkyl; n = 0-2] and their pharmaceutically acceptable salts which are inhibitors of nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease and pain, were prepared E.g., a 4-step synthesis of I.fumarate [X, Y = Cl; Z = H; V = O; W = Bu; R1 = Me; R2 = H] was given. The exemplified compds. I showed IC50 values of < 50 μM against NO synthase.

IT 357415-95-3P 357415-96-4P 357415-97-5P
357416-00-3P 357416-01-4P 357416-02-5P
357416-18-3P 357416-19-4P 357416-24-1P
357416-32-1P 357416-33-2P 357416-36-5P
357416-37-6P 357416-45-6P 357416-46-7P
357416-49-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase)

RN 357415-95-3 CAPLUS

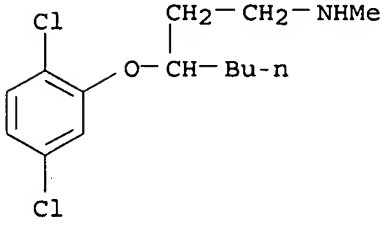
CN 1-Heptanamine, 3-(2,5-dichlorophenoxy)-N-methyl- (9CI) (CA INDEX NAME)



RN 357415-96-4 CAPLUS
CN 1-Heptanamine, 3-(2,5-dichlorophenoxy)-N-methyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

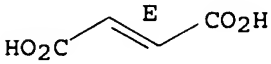
CRN 357415-95-3
CMF C14 H21 Cl2 N O



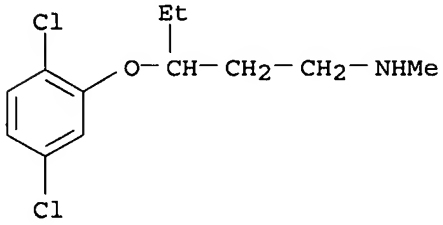
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

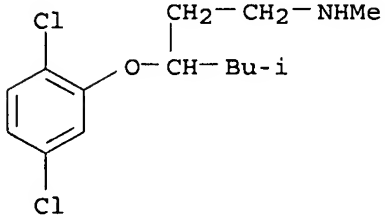


RN 357415-97-5 CAPLUS
CN 1-Pentanamine, 3-(2,5-dichlorophenoxy)-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

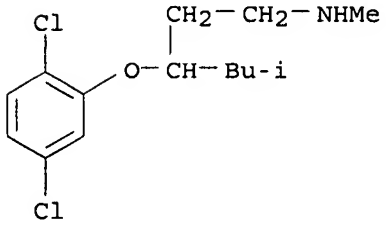
RN 357416-00-3 CAPLUS
CN 1-Hexanamine, 3-(2,5-dichlorophenoxy)-N,5-dimethyl- (9CI) (CA INDEX NAME)



RN 357416-01-4 CAPLUS
CN 1-Hexanamine, 3-(2,5-dichlorophenoxy)-N,5-dimethyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

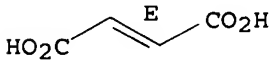
CRN 357416-00-3
CMF C14 H21 Cl2 N O



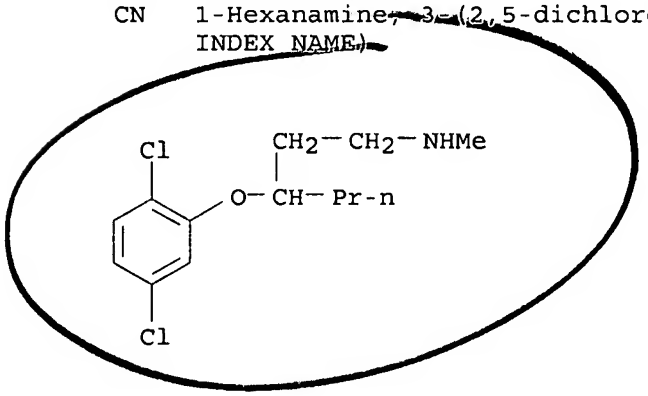
CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

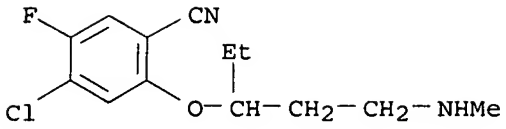


RN 357416-02-5 CAPLUS
CN 1-Hexanamine, 3-(2,5-dichlorophenoxy)-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



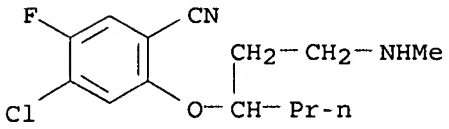
● HCl

RN 357416-18-3 CAPLUS
CN Benzonitrile, 4-chloro-2-[1-ethyl-3-(methylamino)propoxy]-5-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)



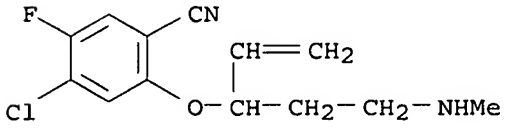
● HCl

RN 357416-19-4 CAPLUS
CN Benzonitrile, 4-chloro-5-fluoro-2-[1-[2-(methylamino)ethyl]butoxy]-, monohydrochloride (9CI) (CA INDEX NAME)



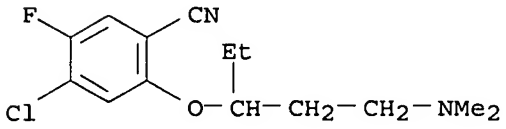
● HCl

RN 357416-24-1 CAPLUS
CN Benzonitrile, 4-chloro-5-fluoro-2-[[1-[2-(methylamino)ethyl]-2-propenyl]oxy]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

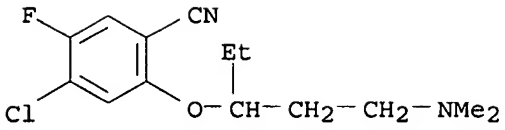
RN 357416-32-1 CAPLUS
CN Benzonitrile, 4-chloro-2-[3-(dimethylamino)-1-ethylpropoxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 357416-33-2 CAPLUS
CN Benzonitrile, 4-chloro-2-[3-(dimethylamino)-1-ethylpropoxy]-5-fluoro-, ethanedioate (9CI) (CA INDEX NAME)

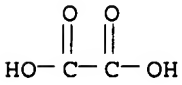
CM 1

CRN 357416-32-1
CMF C14 H18 Cl F N2 O

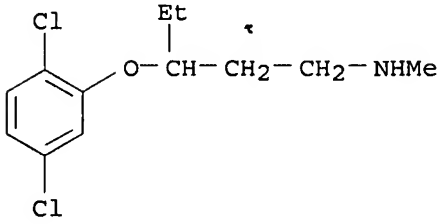


CM 2

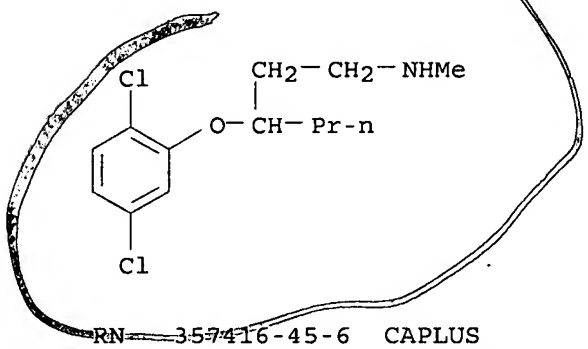
CRN 144-62-7
CMF C2 H2 O4



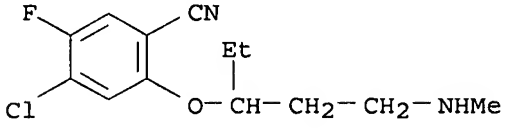
RN 357416-36-5 CAPLUS
CN 1-Pentanamine, 3-(2,5-dichlorophenoxy)-N-methyl- (9CI) (CA INDEX NAME)



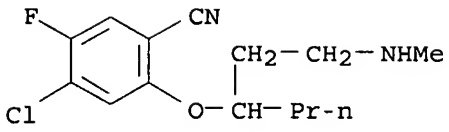
RN 357416-37-6 CAPLUS
CN 1-Hexanamine, 3-(2,5-dichlorophenoxy)-N-methyl- (9CI) (CA INDEX NAME)



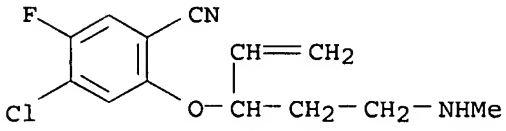
RN 357416-45-6 CAPLUS
CN Benzonitrile, 4-chloro-2-[1-ethyl-3-(methylamino)propoxy]-5-fluoro- (9CI) (CA INDEX NAME)



RN 357416-46-7 CAPLUS
CN Benzonitrile, 4-chloro-5-fluoro-2-[1-[2-(methylamino)ethyl]butoxy]- (9CI) (CA INDEX NAME)

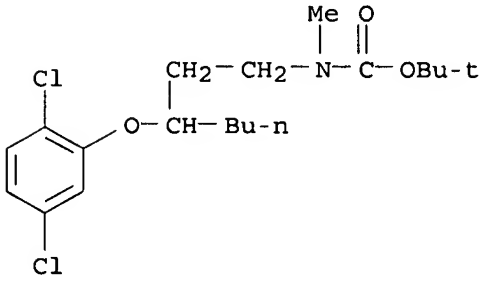


RN 357416-49-0 CAPLUS
CN Benzonitrile, 4-chloro-5-fluoro-2-[[1-[2-(methylamino)ethyl]-2-propenyl]oxy]- (9CI) (CA INDEX NAME)

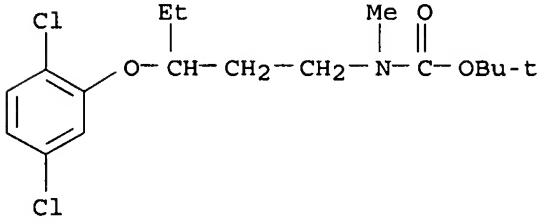


IT 357416-52-5P 357416-54-7P 357416-58-1P
357416-60-5P 357416-72-9P 357416-73-0P
357416-78-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel phenylheteroalkylamines as inhibitors of nitric oxide synthase)

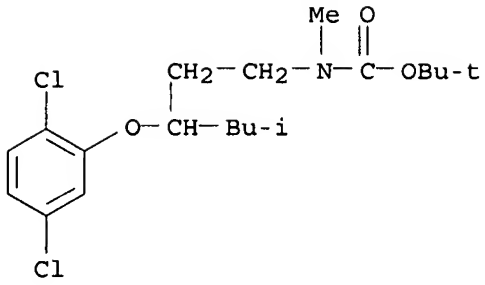
RN 357416-52-5 CAPLUS
CN Carbamic acid, [3-(2,5-dichlorophenoxy)heptyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



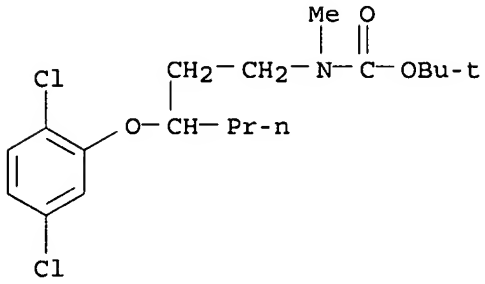
RN 357416-54-7 CAPLUS
CN Carbamic acid, [3-(2,5-dichlorophenoxy)pentyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



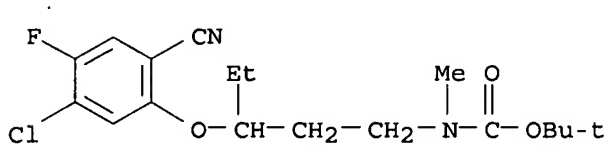
RN 357416-58-1 CAPLUS
CN Carbamic acid, [3-(2,5-dichlorophenoxy)-5-methylhexyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



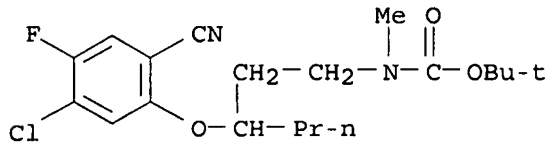
RN 357416-60-5 CAPLUS
CN Carbamic acid, [3-(2,5-dichlorophenoxy)hexyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



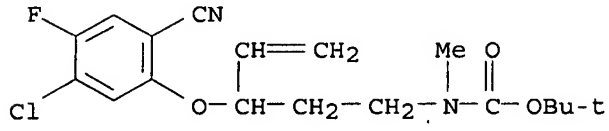
RN 357416-72-9 CAPLUS
CN Carbamic acid, [3-(5-chloro-2-cyano-4-fluorophenoxy)pentyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 357416-73-0 CAPLUS
CN Carbamic acid, [3-(5-chloro-2-cyano-4-fluorophenoxy)hexyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 357416-78-5 CAPLUS
CN Carbamic acid, [3-(5-chloro-2-cyano-4-fluorophenoxy)-4-pentenyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

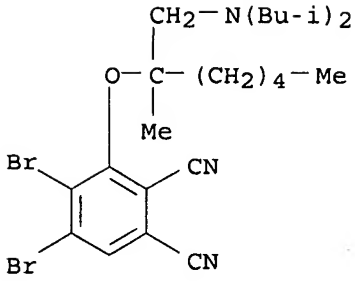
L24 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:334537 CAPLUS
DN 120:334537
TI Phthalocyanine compounds and their usage
IN Itoh, Hisato; Karasawa, Akio; Sugimoto, Kenichi; Oguchi, Takahisa; Aihara, Shin
PA Mitsui Toatsu Chemicals, Inc., Japan; Yamamoto Chemicals, Inc.
SO Eur. Pat. Appl., 67 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 519423	A2	19921223	EP 1992-110218	19920617
	EP 519423	A3	19940309		
	EP 519423	B1	19990303		
	R: DE, FR, GB, NL				
	JP 05171052	A	19930709	JP 1991-338557	19911220
	JP 3016649	B2	20000306		
	CA 2071474	A1	19921220	CA 1992-2071474	19920617
	JP 05295283	A	19931109	JP 1992-160977	19920619
	US 5380842	A	19950110	US 1992-901484	19920622
	US 5695911	A	19971209	US 1995-560130	19951117
PRAI	JP 1991-147310	A	19910619		
	JP 1991-148262	A	19910620		
	JP 1991-338557	A	19911220		
	JP 1992-33031	A	19920220		
	US 1992-901484	A3	19920622		
	US 1994-305317	B1	19940915		

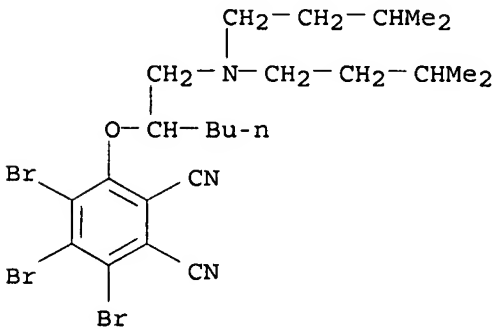
OS MARPAT 120:334537
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. are described by the general formula I (R1, R4, R5, R8, R9, R12, R13, R16 = II, H, or a halogen; R2, R3, R6, R7, R10, R11, R14, R15 = alkyl, alkoxy, alkylthio, alkylamino, dialkyl amino, aryloxy, arylthio, or -COOR17 groups; R17 = substituted or unsubstituted alkyl, hydroxyl, or mercapto groups, H, or a halogen atom; M = a metal atom; X, Z = O or S; R18, R19, R20 = H or alkyl groups; A, B, D = a connecting group; n, l = integers 0-10; m = integer 0-3, 0-2 when used in color filters; q, r, n = integers 0-2; t = integer 0-3, 0-2 when used in color filters; p = 0, 1; and 2 = 0, 1, or 2). Color filters, near-IR absorbing media, and optical recording media employing the compds. are also described.
IT 154434-56-7 154434-57-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in phthalocyanine compound preparation for color filters)
RN 154434-56-7 CAPLUS
CN 1,2-Benzenedicarbonitrile, 3-[[1-[[bis(2-methylpropyl)amino]methyl]-1-methylhexyl]oxy]-4,5-dibromo- (9CI) (CA INDEX NAME)



RN 154434-57-8 CAPLUS
CN 1,2-Benzenedicarbonitrile, 3-[[1-[[bis(3-methylbutyl)amino]methyl]pentyl]oxy]-4,5,6-tribromo- (9CI) (CA INDEX NAME)

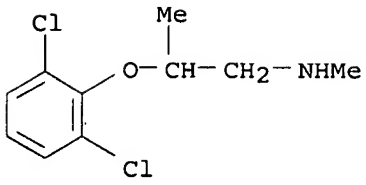


L24 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:493018 CAPLUS
DN 111:93018
TI Protoporphyrin IX tin(IV) and magnesium complexes as photosensitizers for laser-radiation therapy and diagnosis of cancer
IN Fukuda, Yozo; Karasawa, Michito; Uchimoto, Mari; Otani, Takuzo; Aizawa, Katsuo
PA Hamari Chemicals, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63264524	A	19881101	JP 1987-96778	19870420
PRAI JP 1987-96778		19870420		

AB Protoporphyrin IX Sn(IV) complex (I) and protoporphyrin Mg(II) complex (II) are used as photosensitizers for treatment and diagnosis of cancer by laser radiation. A solution of protoporphyrin IX di-Me ester (III) in CH2Cl2 was refluxed with a saturated solution of Sn(OAc)2 in MeOH to give III Sn(IV) complex, which was refluxed in KOH/MeOH to afford I. I at 20 mg/kg i.v. was administered to m-KSA tumor cell-transplanted mice to show 5.47 fluorescence intensity at the tumor tissue and 0.00 relative intensity (normal tissue/tumor tissue) at lung, kidney, and liver, vs. 3.45, 0.45, 0.45, and 0.45 for hematoporphyrin.
IT 1497-11-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as photosensitizer for treatment or diagnosis of cancer by laser radiation)
RN 1497-11-6 CAPLUS
CN 1-Propanamine, 2-(2,6-dichlorophenoxy)-N-methyl-, hydrochloride (9CI) (CA

INDEX NAME)



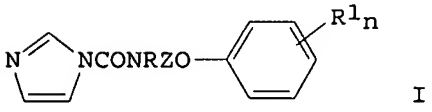
● HCl

L24 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1982:35261 CAPLUS
DN 96:35261
TI Fungicidal carbamoylimidazole compounds
IN Birchmore, Richard John; Brookes, Robert Frederick; Copping, Leonard George; Wells, Wilfred Hase
PA Boots Co. Ltd., UK
SO Brit., 5 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1586998	A	19810325	GB 1978-25644	19780531
	GB 1469772	A	19770406	GB 1973-29535	19730621
	JP 50031047	A	19750327	JP 1974-70743	19740620
	JP 60010003	B	19850314		
	DD 113164	A5	19750520	DD 1974-179314	19740620
	CS 188185	B2	19790228	CS 1974-4365	19740620
	FR 2234293	A1	19750117	FR 1974-21739	19740621
	US 3991071	A	19761109	US 1974-532667	19741213
	ZA 7408037	A	19760128	ZA 1974-8037	19741218
	US 4154945	A	19790515	US 1978-879564	19780221
	CH 635325	A5	19830331	CH 1978-9676	19780915
PRAI	GB 1973-29535	A	19730621		
	US 1974-477734	A2	19740610		
	US 1974-6532667	A3	19741213		
	US 1975-720880	A3	19760907		
	GB 1978-25644	A	19780531		

GI



I

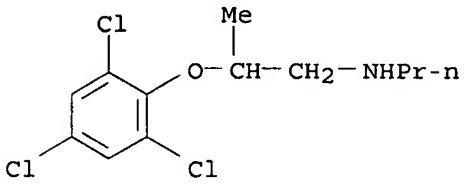
AB The title compds. I (R = alkyl; R1 = H, alkyl, halo; Z = branched alkylene; n = 0-5) and I metal complexes, useful as crop fungicides, were prepared E.g., I (R = Pr, Z = CHMeCH2, R1 = H, n = 1) (II) was prepared from imidazole by treatment with ClCONPrCHMeCH2OPh (dry THF, reflux, 24 h). The fungicidal activities of I were assessed against mildew on barley; 150 ppm II gave >50% control.

IT 80405-86-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation reaction of, with phosgene)

RN 80405-86-3 CAPLUS

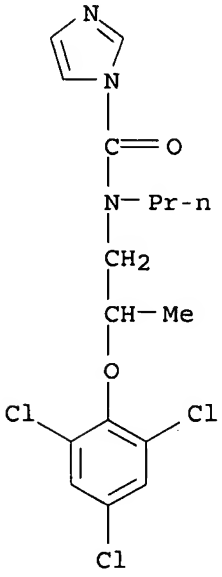
CN 1-Propanamine, N-[2-(2,4,6-trichlorophenoxy)propyl]- (9CI) (CA INDEX NAME)



IT 80405-78-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as fungicide for crops)

RN 80405-78-3 CAPLUS

CN 1H-Imidazole-1-carboxamide, N-propyl-N-[2-(2,4,6-trichlorophenoxy)propyl]- (9CI) (CA INDEX NAME)



L24 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1976:26863 CAPLUS

DN 84:26863

TI 1,3-Dicyano-2,5,6-trichlorobenzene derivatives as fungicides

IN Tamura, Saburo; Katagiri, Kenji; Ishii, Tetsuo; Tamura, Saburo

PA Showa Denko K.K., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

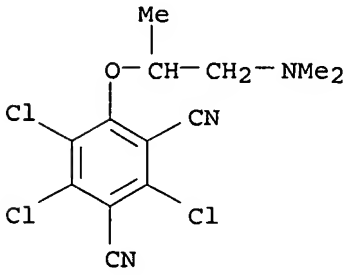
DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 50121424	A	19750923	JP 1974-24837	19740305
	JP 57015562	B	19820331		
PRAI	JP 1974-24837	A	19740305		

OS CASREACT 84:26863
GI For diagram(s), see printed CA Issue.
AB The title compds. I (R = H, alkali metal, alkali earth metal, divalent metal, alkyl, cycloalkyl, substituted alkyl, alkenyl, substituted alkenyl, and Ph) are synthesized and are effective against fungi. Thus, 1,3-dicyano-4-methoxy-2,5,6-trichlorobenzene (II) [57531-87-0] was prepared by treating tetrachloroisophthalonitrile [1897-45-6] with anhydrous methanol [67-56-1]. Thirty-one other I were similarly prepared II (125 ppm) had fungicidal activity against Scleorotinia sclerotiorum, Venturia nashicola, Botrytis cinerea, Trichophyton mentagrophytes, Diaporthe citri, Piricularia oryzae, Pellicularia sasakii, and Alternaria kikuchiana, in vitro.
IT 57532-01-1P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and fungicidal activity of)
RN 57532-01-1 CAPLUS
CN 1,3-Benzenedicarbonitrile, 2,4,5-trichloro-6-[2-(dimethylamino)-1-methylethoxy]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L24 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1973:84247 CAPLUS
DN 78:84247
TI Cardiac 2-alkyl-3-(4-(aminoalkoxy)-3,5-dihalobenzoyl)benzo(b)thiophenes
IN Descamps, Marcel C.; Claeys, Norbert
PA Labaz
SO Ger. Offen., 33 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2230669	A	19721228	DE 1972-2230669	19720623
	GB 1357212	A	19740619	GB 1971-30032	19710625
	BE 784260	A1	19721201	BE 1972-118162	19720601
	FI 54477	C	19781211	FI 1972-1578	19720605
	ZA 7203868	A	19730328	ZA 1972-3868	19720606
	HU 166255	B	19750228	HU 1972-LA799	19720613
	CH 548409	A	19740430	CH 1973-17952	19720621
	CH 549042	A	19740515	CH 1972-9302	19720621
	SE 385482	B	19760705	SE 1972-8187	19720621
	FR 2143250	A1	19730202	FR 1972-22480	19720622
	NL 7208703	A	19721228	NL 1972-8703	19720623
	SU 453844	A3	19741215	SU 1972-1800666	19720623

	CA 959492	A1	19741217	CA 1972-145600	19720623
	JP 48044248	A	19730626	JP 1972-63621	19720624
	ES 404252	A1	19750601	ES 1972-404252	19720624
	AT 312597	B	19740110	AT 1972-5459	19720626
PRAI	GB 1971-30032	A	19710625		

GI For diagram(s), see printed CA Issue.

AB The hydrochlorides or oxalates of about 50 title compds. (I, n = 1-5; R = H or C1-4 alkyl; R2 = H or Me; R3 = Br, Cl, or iodo; R4 = C1-4 alkyl; or NR24 = 1-pyrrolidinyl, piperidino, or 1-perhydroazepinyl), used as drugs with antiadrenergic activities in the treatment of tachycardia and angina pectoris, were prepared from 3-(p-hydroxybenzoyl)benzo[b]thiophenes by halogenation to give the 3,5-dihalo-4-hydroxybenzoyl derivs. and reaction of these with ClCHR2(CH2)nNR24, MeC6H4SO3CHR2(CH2)nNR24, or with BrCHR2(CH2)nBr and R24NH. Thus, 3-anisoyl-2-ethylbenzo[b]thiophene was treated with pyridine-HCl 1 hr at 220° to give 94% 2-ethyl-3-(p-hydroxybenzoyl)benzo[b]thiophene (II). II, treated with AcONa in MeOH, was brominated with Br in AcOH to give 78.8% 2-ethyl-3-(3,5-dibromo-4-hydroxybenzoyl)benzo[b]thiophene (III). III and K2CO3 were heated in DMF 1 hr and then 90 min with Br(CH2)3Br to give IV (n = 2, R = Et, R2 = H, R3 = Br), which was treated with Pr2NH in DMF and C6H6 2 hr at reflux to give after addition of HCl 39% I.HCl (n = 2, R = Et, R2 = H, R3 = Br, R4 = Pr). Refluxing IV and K2CO3 in aqueous ClCH2CH2Cl 1 hr and with addnl. ClCH2CH2NPr2.HCl 3 hr gave, after addition of HCl, 40% I.HCl (n = 1, R = Et, R2 = H, R3 = Br, R4 = Pr).

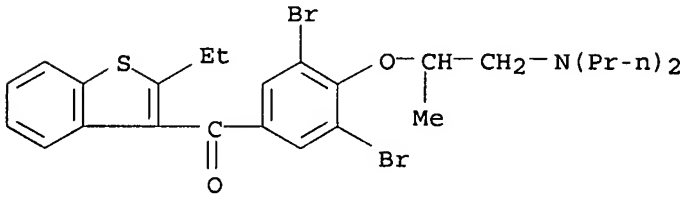
IT 39620-85-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 39620-85-4 CAPLUS

CN Methanone, [3,5-dibromo-4-[2-(dipropylamino)-1-methylethoxy]phenyl](2-ethylbenzo[b]thien-3-yl)-, ethanedioate (9CI) (CA INDEX NAME)

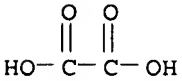
CM 1

CRN 47701-69-9
CMF C26 H31 Br2 N O2 S



CM 2

CRN 144-62-7
CMF C2 H2 O4



L24 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1971:448675 CAPLUS

DN 75:48675

TI Fungicidal alkyl aminoalkyl pentachlorophenyl ethers

IN Seki, Shigeo; Matsuni, Tomio

PA Meiji Confectionary Co. Ltd.
SO U.S., 4 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3567723	A	19710302	US 1967-639063	19670517

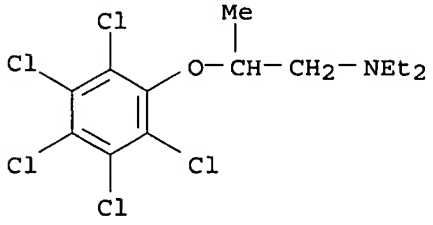
PRAI JP 1966-32063 A 19660521

AB The title ethers Cl5C6OQNRR1 (I, Q = alkylene; R1,R2 = alkyl, aralkyl; R1, Et R2; NR1R2 = pyrrolidino, piperidino, morpholino) were produced by reacting excess Cl5C6OM (M = alkali metal ion) with R1R2NAX.HX (X = Cl, Br) in a lower alkyl alc. or dioxane. Thus Cl5C6ONa and Bu2NCH2CH2Cl.HCl refluxed 3 hr in alc. gave I (R1 = R2 = Bu, Q = CH2CH2). Similarly were obtained I (Q and NR1R2 given): (CH2)2, piperidino; (CH2)2, morpholino; (CH2)2, N(CH2Ph)2; (CH2)3, NMe2; CHMeCH2, NEt2; Similarly was prepared I [Q = (CH2)2, (NR1R2) = piperidino].HCl salt. I in the form of saccharin salts sprayed in 1% MeOH solution on rice plants showed marked fungicidal activity against rice blast fungi with negligible phytotoxicity. The LD50 toxicity to fish was in excess of 2.5 or 5.0 ppm of saccharin salts.

IT 24773-45-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24773-45-3 CAPLUS

CN Propylamine, N,N-diethyl-2-(pentachlorophenoxy)-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

L24 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1970:12361 CAPLUS

DN 72:12361

TI Alkylaminoalkyl pentachlorophenyl ether

IN Seki, Isao; Matsuno, Tomio

PA Meiji Confectionary Co., Ltd.

SO Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXXAD

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 44026453	B4	19691106	JP	19660521

GI For diagram(s), see printed CA Issue.

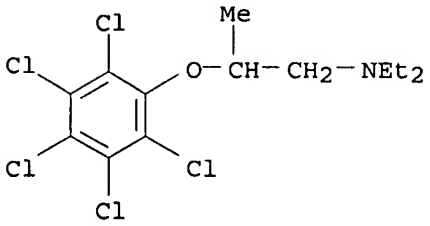
AB Manufacture of I, useful as an antifungal substance, is described. In an example, a mixture of 72 g. pentachlorophenol (Na salt) and 228 g. β-(dibutylamino)ethyl chloride in 300 cc. EtOH is refluxed 3 hrs., the mixture evapd in vacuo, the residue stirred with 300 cc. H2O and 10 g. NaOH, the mixture extracted with PhMe, the extract evaporated, and the residue cooled

after addition of iso-PrOH to give 35 g. I [R = Bu2N, X = (CH2)2], m. 30-1°. Similarly prepared are the following I (R, X, and m.p. given): piperidino, (CH2)2, 69-70° (hydrochloride m. 209-10°); morpholino, (CH2)2, 89-9.5°; (PhCH2)2N, (CH2)2, 63-4°; Me2N, (CH2)3, (hydrochloride, m. 196-7°); Et2N, CHMeCH2; hydrochloride m. 172.5-3.5°.

IT 24773-45-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 24773-45-3 CAPLUS

CN Propylamine, N,N-diethyl-2-(pentachlorophenoxy)-, hydrochloride (8CI) (CA INDEX NAME)



● HCl

L24 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1968:21633 CAPLUS

DN 68:21633

TI Synthesis and preliminary pharmacological investigation of 2-methyl-2-(2,6-dichlorophenoxy)-1-dimethylamino)propane hydrochloride

AU De Marchi, Franco; Torrielli, M. V.; Cossa, Gian A.

CS "Schiapparelli" S.p.A., Turin, Italy

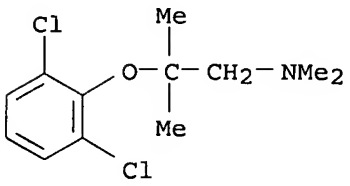
SO Farmaco, Edizione Scientifica (1967), 22(8), 641-50
CODEN: FRPSAX; ISSN: 0430-0920

DT Journal

LA Italian

AB A mixture of 150 g. 2,6-dichlorophenol, 250 g. NaOH in 960 ml. Me2CO was treated with 150 g. CHCl3, refluxed 5 hrs. with stirring, evaporated, and the residue dissolved in H2O. The resulting solution, washed with Et2O and acidified with HCl, gave 119 g. 2-methyl-2-(2,6-dichlorophenoxy)propionic acid (I), m. 125°, in 52% yield. I gave with SOCl2 the corresponding acid chloride (II), b0.02 90°, in 93% yield. A solution of 42 g. II in 150 ml. CH2Cl2 was added in 30 min. at 20° to a stirred solution of 14.6 g. Me2NH in 150 ml. CH2Cl2. After an addnl. stirring 90 min. at 20°, the mixture was refluxed 90 min., the solvent evaporated in vacuo, and the residue dissolved in 350 ml. Et2O. The ethereal solution washed with 2N HCl, H2O, NaHCO3 solution, dried and evaporated gave 40.2 g. 2-methyl-2-(2,6-dichlorophenoxy)-N,N-dimethylpropionamide (III), b0.07 105-10°, in 93% yield. II (38 g.) was reduced in dry Et2O with 0.24M LiAlH4 in Et2O. The mixture was refluxed 15 hrs., cooled at 5°, treated with AcOEt, H2O, 20% NaOH solution, and H2O; the Et2O layer was dried on K2CO3 and evaporated and the residue distilled to yield 29 g. oil, b0.04 80°, which dissolved in 350 ml. Et2O gave with 10% alc. HCl 32 g. 2-methyl-2-(2,6-dichlorophenoxy)-1-dimethylaminopropane-HCl (IV), m. 191-3°, in 78% yield. The pharmacol. properties of IV, especially its local anesthetic activity, were examined and compared with those of 2-(2,6-dichlorophenoxy)-1-dimethylaminoethane-HCl.

IT 14443-45-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and pharmacol. properties of)
RN 14443-45-9 CAPLUS
CN 1-Propanamine, 2-(2,6-dichlorophenoxy)-N,N,2-trimethyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L24 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:403170 CAPLUS
DN 63:3170
OREF 63:547f-h,548a-c
TI Antidepressive phenoxyalkylamines
IN Tedeschi, David H.
PA Smith Kline & French Laboratories
SO 17 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR M3075		19650222	FR	
	BE 640617			BE	
	GB 1014348			GB	
	NL 302148			NL	
	US 3205136		19650907	US 1962-246672	19621224
PRAI	US		19621224		

OS MARPAT 63:3170
GI For diagram(s), see printed CA Issue.
AB The title compds. of general formula I are prepared by condensation of the appropriate phenol with an alkylamine halide or with an α-haloaminoalkylamide, followed by reduction Thus, to a suspension of 1.9 g. NaH in 50 ml. anhydrous toluene a solution of 8.8 g. 2,6-dimethylphenol in 60 ml. anhydrous toluene is added rapidly, the mixture stirred and refluxed 1 hr., cooled, a solution of 15 g. N,N-dimethyl-α-bromopropionamide added, the mixture refluxed with stirring 12 hrs., filtered, the filtrate washed with 10% NaOH and H2O, dried, and concentrated in vacuo, and the residue distilled to give N,N-dimethyl-α-(2,6-dimethylphenoxy)propionamide (II), b0.6-0.8 110-23°. To a suspension of 11.7 g. LiAlH4 in 250 ml. anhydrous Et2O a solution of 25.3 g. II in 250 ml. anhydrous Et2O is added giving an exothermic reaction. Et2O (300 ml.) is added, the mixture refluxed with stirring 2.5 hrs., stirred at room temperature for 61 hrs., over 15 min. a solution of 24.3 ml. EtOAc in 50 ml. Et2O added, followed by 22.5 ml. H2O over 20 min., and the mixture stirred at room temperature 1 hr., filtered, dried, and concentrated, to give N,N-dimethyl-2-(2,6-dimethylphenoxy)propylamine, b0.3 70-4°; HCl salt m. 161.5-2.5° (EtOH-Et2O). Alternatively, a solution of 81.5 g. 2,6-dichlorophenol in 300 ml. anhydrous toluene is added slowly to 12.5 g. NaH in 200 ml. toluene over 20 min., refluxed 1 hr., and cooled. A solution

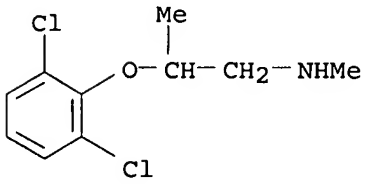
of 144.1 g. β-dimethylaminoethyl chloride in anhydrous toluene is added over 1 hr., the mixture refluxed with stirring 8 hrs., cooled, and treated with 150 ml. H2O and 250 ml. 3M HCl. The toluene layer is extracted with 250 ml. 3M HCl, and the acid extract extracted with Et2O and made alkaline with 40% NaOH.

The amine is taken up in Et2O, the aqueous layer extracted with Et2O, dried, evaporated, and the residue distilled to give N,N-dimethyl-2-(2,6-dichlorophenoxy)ethylamine, b0.8-0.9 90-2° (HCl salt m. 172-4°). Also prepared were (b.p. and m.p. HCl salt given): N,N-dimethyl-2-(2,6-dichlorophenoxy)propylamine, -, 175.5-7.5°; N,N-dimethyl-3-(2,6-dimethylphenoxy)propylamine, b0.5-0.75 104-7°, 170-2°; N,N-dimethyl-2-(2,4-dichlorophenoxy)ethylamine, b0.35. 94-107°, 125.5-7.5°; N,N-dimethyl-2-(2,6-diisopropylphenoxy)ethylamine, b0.3 84-8°, 207-10.5°; N,N-dimethyl-2-(2,6-dibromophenoxy)ethylamine, b0.35-0.6 106-16°, 201-3°; 2-(2,6-dichlorophenoxy)-N,N,1-(trimethyl)ethylamine, b0.25 90-1°, 196-7°; N-[2(2,6-dichlorophenoxy)ethyl]pyrrolidine, b0.15 118-22°, 181.5-2.5°; N-[2-(2,6-dichlorophenoxy)ethyl]piperidine, b0.15 121-4°, 185-6°; N-methyl-2-(2,6-dichlorophenoxy)propylamine, b0.15 96-116°, 156-7°; N,N-dimethyl-2-[3,5-bis(trifluoromethyl)phenoxy]ethylamine, b21 110°, 193-3.5°; N,N-dimethyl-2-(2,6-dimethoxyphenoxy)ethylamine, b0.7-0.85 107-15°, 186.5-7.5°; N,N-dimethyl-2-(2-chlorophenoxy)propylamine, b1 75°, 134.5-36°; and N,N-dimethyl-2-phenoxypropylamine, b0.5-0.6 54-9°, 146-7°. The addition compounds with physiologically acceptable acids are useful antidepressants, especially the salts of N,N-dimethyl-2-(2,6-dichlorophenoxy)propylamine.

IT 1485-39-8, Propylamine, 2-(2,6-dichlorophenoxy)-N-methyl- 1485-45-6, Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl-, hydrochloride 1497-11-6, Propylamine, 2-(2,6-dichlorophenoxy)-N-methyl-, hydrochloride
(nuclear magnetic resonance of, substituent effect in)

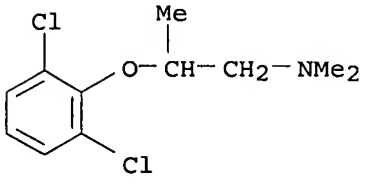
RN 1485-39-8 CAPLUS

CN Propylamine, 2-(2,6-dichlorophenoxy)-N-methyl- (7CI, 8CI) (CA INDEX NAME)



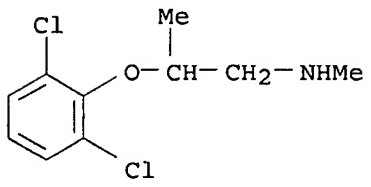
RN 1485-45-6 CAPLUS

CN Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



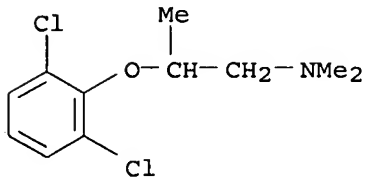
● HCl

RN 1497-11-6 CAPLUS
CN 1-Propanamine, 2-(2,6-dichlorophenoxy)-N-methyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 1485-45-6P, Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl-, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 1485-45-6 CAPLUS
CN Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl-, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

L24 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1964:16578 CAPLUS
DN 60:16578
OREF 60:2893c-d
TI Chloromethyl 5-nitro-2-furyl ketone
IN Gever, Gabriel
PA Norwich Pharmacal Co.
SO 1 p.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3111530		19631119	US 1962-219731	19620827
	BE 636669			BE	
	DE 1210885			DE	
	FR 1367885			FR	
	NL 296646			NL	
PRAI	US		19620827		

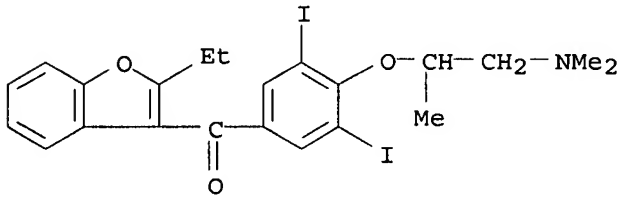
GI For diagram(s), see printed CA Issue.
AB A mixture of 5 g. bromomethyl 5-nitro-2-furyl ketone and 125 ml. concentrated HCl
was heated, with stirring, on a steam bath at 80° 10 min., then

cooled to give the title compound (I), 60% yield, m. 96-7° (CCl4). I is a disinfectant and an antiseptic. The reactants here lack the insidious toxicity of those used in the past.

IT 95940-21-9
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 95940-21-9 CAPLUS

CN Ketone, 4-[2-(dimethylamino)-1-methylethoxy]-3,5-diiodophenyl 2-ethyl-3-benzofuranyl, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L24 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1964:16577 CAPLUS

DN 60:16577

OREF 60:2892g-h,2893a-c

TI 2-Alkyl-3-[4-[2-aminoethoxy)benzoyl]benzofuran hydrochlorides

PA Societe Belge de l'Azote et des Produits Chimiques de Marly, S.A.

SO 16 pp.

DT Patent

LA Unavailable

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 1339389		19631004	FR 1962-916270	19621122
	BE 625039			BE	
	FR M2280			FR	
	GB 995367			GB	
	US 3248401		1966	US	
PRAI	DE		19611124		

OS MARPAT 60:16577

GI For diagram(s), see printed CA Issue.

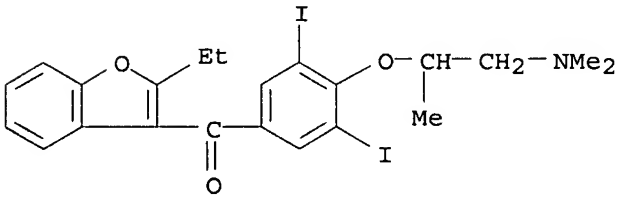
AB 2-Alkyl-3-(4-hydroxybenzoyl)benzofurans are treated with R2NCH2CH2Cl to give the title compds., which have therapeutic properties. Thus, 97 g. 2-ethyl-3-(4-hydroxybenzoyl)benzofuran is dissolved in 500 ml. dry PhMe at 60°, a solution of 8.4 g. Na in 200 ml. MeOH added, the mixture heated at .apprx.100° and cooled to .apprx.50°, a solution of 76 g. Et2NCH2CH2Cl.HCl in PhMe added, the mixture heated .apprx.2 hrs. at 90°, allowed to cool, kept overnight, and extracted with HCl, the exts. washed with ether, made alkaline with NaOH, and extracted 3 times with ether, the extract treated with HCl in ether, the mixture kept several hrs. and decanted, the residue taken up in 500 ml. boiling EtOAc, and the solution cooled and kept overnight at 0° to precipitate 110 g. 2-ethyl-3-[4-(2-N-diethylaminoethoxy)benzoyl]benzofuran-HCl, m. 114°. Similarly prepared are the following I (X, R, R', and m.p. given): H, Me, Et, --; H, (R2N=) piperidino, Et, 122° (EtOAc); H, (R2N =) morpholino, Et, 198-200° (MeOH-Me2CO); H, Et, neohexyl, 172° (EtOAc-ether); H, (R2N=) pyrrolidinyl, Et, 174° (MeOH-EtOAc); H, Et, Bu, 102° (EtOAc-ether); iodine, Et, Bu, 156°; iodine, Et, Et, 152° (Me2CO); iodine, Et, Pr, 166° (MeOH-Me2CO); iodine, Et, iso-Pr, 172° (Me2CO-EtOAc); iodine, Et, Me, 153° (Me2CO);

iodine, Et, neopentyl, 169° (MeOH-Me2CO);iodine, Et, neohexyl, 150° (Me2CO-EtOAc); iodine, Et, Am, 155° (EtOAc); Br, Et, Et, 150° (EtOAc-ether); iodine, (R2N =) piperidino, Et, 172-3° (Me2CO-EtOAc); iodine, Pr, Et, 170° (MeOH-AcEt); iodine, Me, Et, 170° (Me2CO-EtOAc); iodine, (R2N=) pyrrolidinyl, Et, 189° (MeOH-Me2CO). Also prepared are 2-ethyl-3-[3,5-diiodo-4(α-methyl-β-N-piperidinoethoxy)benzoyl]benzofuran-HCl, m. 176° (Me2CO); 2-ethyl-3- [3,5-diiodo-4(α-methyl-β-N-dimethylamino-ethoxy)benzoyl]benzofuran-HCl, m. 178° (MeOH-Me2CO); and 2-ethyl-3-[3,5-diiodo-4-(β-N-diethylaminoethoxy)benzoyl]benzofuran (II)nitrate, m. 129° (Me2CO-EtOAc); II acid sulfate m. 154° (Me2CO-EtOAc).

IT 95940-21-9P, Ketone, 4-[2-(dimethylamino)-1-methylethoxy]-3,5-diiodophenyl 2-ethyl-3-benzofuranyl, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 95940-21-9 CAPLUS

CN Ketone, 4-[2-(dimethylamino)-1-methylethoxy]-3,5-diiodophenyl 2-ethyl-3-benzofuranyl, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L24 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1963:485028 CAPLUS

DN 59:85028

OREF 59:15803g-h,15804a

TI A new local anesthetic with a long duration of action

AU Hey, P.; Willey, G. L.

CS Smith, Kline & French, Hertfordshire, UK

SO Nature (London, United Kingdom) (1963), 198, 390-1
CODEN: NATUAS; ISSN: 0028-0836

DT Journal

LA Unavailable

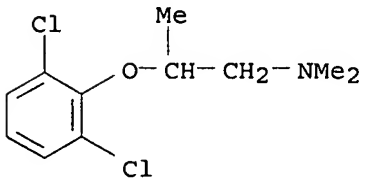
AB 2-Phenoxyethyldialkylamines of the type shown in the general formula 2,6-R2C6H3OCH(R1)CH(R2)N(R3)R4 were given as the hydrochloride or hydrobromide and tested for anesthesia by the Bulbring and Wajda intracutaneous wheal method in guinea pigs. Observations were made every 5 min. for 30 min. and then at 30-min. intervals for up to 5 hrs. The durations of the anesthetic effect produced by 1% were compared with lignoeaine-HCl (I). When R1 and R2 are H, the dimethylamine compds. have a longer anesthetic effect than the corresponding diethylamino compds., and the R = Cl gives more prolonged anesthetic effects than does R = Me. Replacement of H by Me in position R1 or R2 does not affect potency, but the duration of the anesthetic effect is reduced. The compound (II) in which R = Cl, R1 = H, R2 = H and R2 = R3 = Me causes complete anesthesia for 1 hr. and some degree of anesthesia for 4 hrs., in contrast to I with which anesthesia is complete for only about 10 min. and disappears within 1 hr. On topical application to the rabbit cornea, II produces anesthesia for about twice as long as I when equal concns. are used. A 1% solution of II has no apparent effect on capillary permeability, whereas 1% I produces a small effect. Two % concns. of both drugs cause a similar degree of

capillary damage. Intravenous injection of II (1-5 mg./kg.) causes a fall in the arterial blood pressure of anesthetized rats or cats; toxic doses (10-25 mg./kg.) produce respiratory and heart failure. II depresses the isolated rabbit heart preparation and is slightly more active than I in this respect. I and II are equivalent in increasing the blood flow through the hind limb of anesthetized cats. The acute intravenous L.D.50 in male mice of II is 29 mg./kg., compared with 20 mg./kg. subcutaneously and 290 mg./kg. orally. There is no significant difference in toxicity to male and female mice.

IT 22196-56-1, Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl- (as anesthetic)

RN 22196-56-1 CAPLUS

CN Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl- (7CI, 8CI) (CA INDEX NAME)



L24 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1963:431353 CAPLUS

DN 59:31353

OREF 59:5668g-h,5669a

TI A spinal anesthetic with long duration of action

AU Davies, F. Glyn

CS Univ. Oxford, UK

SO Nature (London, United Kingdom) (1963), 198(4878), 390
CODEN: NATUAS; ISSN: 0028-0836

DT Journal

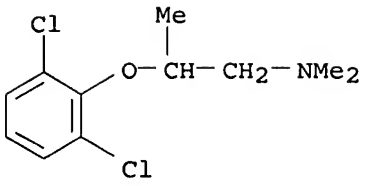
LA Unavailable

AB Clun ewes at 9-10 months of age and a weight of 30-39 kg. having a mean crown-rump length of 78 cm. were used. Spinal or epidural injections of 2-(2,6-dichlorophenoxy)ethyldimethylamine-HBr (I) were made through the lumbosacral spaces. Doses were used which anesthetized the spinal nerves from lumbar vertebra 2-3 caudally. Lignocaine (II) and I (20 mg./ml.) were administered as the hyperbaric solution in 65% glucose; 1.5 ml. intrathecally or 4.5 ml. epidurally of either solution was injected at intervals of a week. The index of sensory block was the withdrawal of hind-limbs in response to pin pricks below the hock. Loss of tonus and inability to move the limbs on change of posture assessed motor block. The duration of anesthesia of I was more than twice that of II regardless of means of application. There was no significant difference in the time of onset of anesthesia after injection. After intrathecal injection, II did not abolish limb movements completely in some of the lambs but I caused complete loss of tonus. All ewes fully recovered after both anesthetics. There were no neurological abnormalities afterwards.

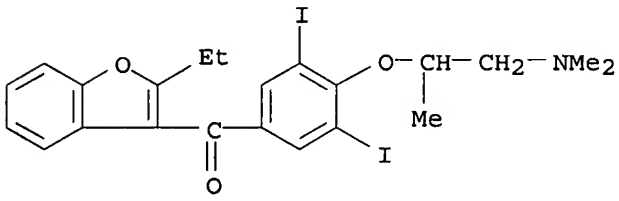
IT 22196-56-1, Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl- (as anesthetic)

RN 22196-56-1 CAPLUS

CN Propylamine, 2-(2,6-dichlorophenoxy)-N,N-dimethyl- (7CI, 8CI) (CA INDEX NAME)

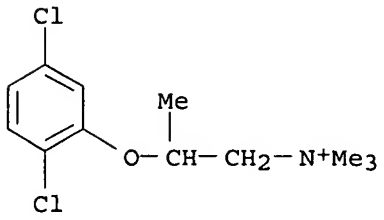


L24 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1963:22719 CAPLUS
DN 58:22719
OREF 58:3788d-e
TI The benzofuran series. VI. The coronary-dilating activity of alkyl and aminoalkyl derivatives of 3-benzoylbenzofuran
AU Deltour, G.; Binon, F.; Tondeur, R.; Goldenberg, C.; Henaux, F.; Sion, R.; Deray, E.; Charlier, R.
CS Produits Chim. Marly, Brussels, Belg.
SO Archives Internationales de Pharmacodynamie et de Therapie (1962), 139, 247-54
CODEN: AIPTAK; ISSN: 0003-9780
DT Journal
LA French
AB cf. CA 56, 4049i. The title activity of approx. 40 derivs. of benzoyl-3-benzofuran (I) was determined on the isolated rabbit heart. Structural formulas of the compds. are indicated. They contained the I nucleus in the form of a substituted 2-alkyl-3-(4-hydroxybenzoyl)benzofuran (II) structure. Physico-chemical alterations of the basic structure (polarity, electronegativity, and ratios between water solubility and liposoly.) are considered in relation to pharmacodynamic activity. Besides substitutions with alkyl and related groups, the effects of Br or iodine substitution in the 3' and 5' positions were determined The compds. showed wide differences in coronary-dilating action. Changes in the alkyl chain in the 2-position and certain substitutions in the 4'-position (particularly by the β-N-diethylaminoethyl radical) considerably increased the action.
IT 95940-20-8, Ketone, 4-[2-(dimethylamino)-1-methylethoxy]-3,5-diiodophenyl 2-ethyl-3-benzofuranyl
(heart circulation response to)
RN 95940-20-8 CAPLUS
CN Ketone, 4-[2-(dimethylamino)-1-methylethoxy]-3,5-diiodophenyl 2-ethyl-3-benzofuranyl (7CI) (CA INDEX NAME)



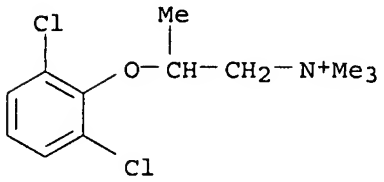
L24 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:82068 CAPLUS
DN 54:82068
OREF 54:15683b-d
TI A series of 2,6-disubstituted phenoxyethyltrimethylammonium bromides with true sympatholytic properties
AU McLean, R. A.; Geus, R. J.; Mohrbacher, R. J.; Mattis, P. A.; Ullyot, G. E.
CS Smith, Kline & French Labs., Philadelphia, PA

SO Journal of Pharmacology and Experimental Therapeutics (1960), 129, 11-16
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA Unavailable
AB 2,6-Dimethyl- and 2,6-dichlorophenoxyethyltrimethylammonium bromides and their α- and β-Me derivs. were synthesized and studied for autonomic effects. The muscarinic-stimulant activity of the parent compds. was reduced by α-methylation (on C adjacent to N) and eliminated by β-methylation. Sympathetic-inhibitor potency, revealed by relaxation of the nictitating membrane in anesthetized cats, was reduced by β-methylation. Tests with autonomic drugs and nerve action potential recordings indicated that the characteristic inhibition produced by the unsubstituted and the β-substituted congeners is selective for the terminal sympathetic nerve endings.
IT 108900-98-7
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 108900-98-7 CAPLUS
CN [2-(2,5-Dichlorophenoxy)propyl]trimethylammonium bromide (6CI) (CA INDEX NAME)



● Br^-

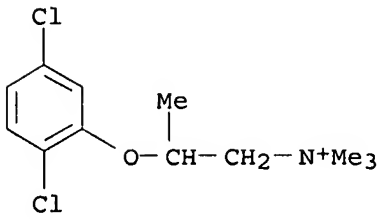
IT 857012-43-2, Ammonium, [2-(2,6-dichlorophenoxy)propyl]trimethyl-, bromide
(as sympatholytic substance)
RN 857012-43-2 CAPLUS
CN Ammonium, [2-(2,6-dichlorophenoxy)propyl]trimethyl-, bromide (6CI) (CA INDEX NAME)



● Br^-

L24 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1960:82067 CAPLUS
DN 54:82067
OREF 54:15682i,15683a-b
TI Antimetabolites and fetal development
AU Richter, R. H. H.
CS Univ. Bern, Switz.

SO Helvetica Physiologica et Pharmacologica Acta (1960), 18, C46-C47
CODEN: HPPAAL; ISSN: 0367-6242
DT Journal
LA German
AB In pregnant rats isoriboflavine (antivitamin B2), 8 mg./day added to a low vitamin B2 diet for 3 weeks caused damage to the fetuses in one strain of rats but not in several others. In Wistar rats 4-hydroxythiamine chloride (antivitamin B1), 10 mg./day added to the normal diet for the 1st 15 days of pregnancy, resulted in death and resorption of the fetuses in 5 of 7 rats. 4-Deoxypyridoxine (antivitamin B6), 5 mg./day added to normal diet, caused no significant damage to the fetuses. When 3-(3-keto-17β-hydroxy-19-norandrost-4-ene-17α-yl)propionic acid lactone, which has been reported to have a progestative action (cf. CA 53, 6435c), was injected intramuscularly in oil, 3 mg./kg./day for the 1st 15 days of pregnancy in Wistar rats, about 26% of the fetuses died and were partly or completely resorbed.
IT 108900-98-7
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 108900-98-7 CAPLUS
CN [2-(2,5-Dichlorophenoxy)propyl]trimethylammonium bromide (6CI) (CA INDEX NAME)



● Br^-

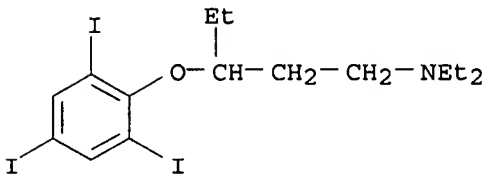
L24 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1943:37587 CAPLUS
DN 37:37587
OREF 37:5995i,5996a-c
TI Effect of aromatic iodine compounds on the tubercle bacillus
AU Saz, Arthur K.; Johnston, Frank R.; Burger, Alfred; Bernheim, Frederick
SO American Review of Tuberculosis (1943), 48, 40-50
CODEN: ARTUA4; ISSN: 0096-0381
DT Journal
LA Unavailable
AB Attention is called to a group of compds. that have marked effects in low concns. on the metabolism and growth of the tubercle bacillus. A twelve-day test involving the weighing of the omentum after i.p. injection in guinea pigs of tubercle bacilli is suggested for determining the effect of these drugs.
The compds. tested were (1) 2,3,5-triiodobenzoic acid, (2) 2,4,6-triiodobenzoic acid, (3) 3,5-diiodo-2-hydroxybenzoic acid, (4) 3,5-diiodo-4-hydroxybenzoic acid, (5) sodium 2,4,6-triiodophenoxyacetate (B 14), (6) 2,4,6-triiodophenol (B 29), (7) 1-diethylamino-2-(2,4,6-triiodophenoxy) ethane-HCl (B 9), (8) 1-diethylamino-3-(2,4,6-triiodophenoxy)propane-HCl (B 7), (9) 3-(2,4,6-triiodophenoxy)-1-diethylaminopentane-HCl (B 30), (10) 3,4,5-triiodobenzenesulfonic acid, (11) 2,3,5-triiodobenzenesulfonic acid, (12) 2,4,5-triiodobenzenesulfonic acid, (13) sozoiodolic acid. Whether pos. results with the test suggested would be an indication of therapeutic action in human tuberculosis is not known. B 9 can be considered relatively nontoxic although it causes some

weight loss in guinea pigs; 2,3,5-triiodobenzoic acid which gave neg. results in the guinea-pig test is tolerated in large doses by human subjects, so that it, as well as B 9, may warrant a therapeutic trial in selected cases.

IT 756865-34-6P, Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, HCl
RL: PREP (Preparation)
(preparation of)

RN 756865-34-6 CAPLUS

CN Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, HCl (4CI) (CA INDEX NAME)



● HCl

L24 ANSWER 21 OF 22 CAPLUS

AN 1941:35078 CAPLUS

DN 35:35078

OREF 35:5471i,5472a-f

TI Arsonium, compounds. III

AU Blicke, F. F.; Safir, S. R.

SO Journal of the American Chemical Society (1941), 63, 1493-6
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

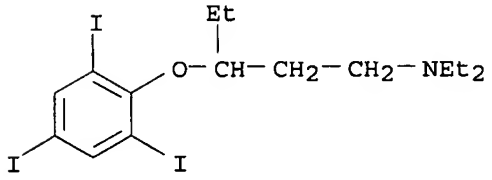
AB cf. C. A. 35, 2123.3. PhMe3AsI with Ag2O in H2O, followed by neutralization with HNO3, gives 88% of PhMe3AsNO3 (I), m. 194-6°. Addition of 5 g. of I to a cold mixture of 2.5 cc. HNO3 (d. 1.6) and 5.5 cc. concentrated H2SO4 and heating on the steam bath for 10 min. give 5 g. of trimethyl-3-nitrophenylarsonium nitrate, m. 278-9° (decomposition); aqueous NaI gives a quant. yield of the iodide, m. 286-90° (decomposition), which with Ag2O, followed by HCl, gives the chloride (II), m. 263-70° (decomposition). Reduction of 10 g. II in 150 cc. AcOH with 38 g. SnCl2.2H2O, the mixture being saturated with HCl, and reaction of the precipitate in 100 cc. H2O with 60 cc. 20% NaOH and 20 g. NaI give 8 g. of trimethyl-3-aminophenylarsonium iodide, m. 175-6° (Ac derivative, m. 242-6° (decomposition)); the chloride (III) m. 243-4° (decomposition) and its Ac derivative m. 256-8° (decomposition). The diazo reaction with 4.2 g. III in 75 cc. H2O and 2.5 cc. concentrated H2SO4, with final heating on the water bath and reaction of the neutral solution with a few drops of HI and 20 g. NaI give 8 g. of trimethyl-3-hydroxyphenylarsonium iodide, m. 208-11° (decomposition). 4-BrC6H4AsMe2 and MeI, heated 12 hrs. on the water bath, give 96% of trimethyl-4-bromophenylarsonium iodide, m. 253-5° (decomposition); the nitrate (IV) m. 163-5°. Nitration of 5 g. IV with 3 cc. HNO3 and 7 cc. H2SO4, with heating for 0.5 hr. on the steam bath, gives 88% of trimethyl-3-nitro-4-bromophenylarsonium nitrate, m. 176-81° (decomposition); the bromide (V) m. 255-75° (decomposition). Reduction of V and treatment of the product with NaOH and then with NaI give trimethyl-3-amino-4-bromophenylarsonium iodide, m. 235-7°. Boiling 2.2 g. of V and 0.7 g. KOH in 15 cc. of H2O for 1 hr. and neutralization with HBr give 1.8 g. of trimethyl-3-nitro-4-

hydroxyphenylarsonium bromide (VI), m. 269-71° (decomposition); the nitrate m. 225°. Reduction of 10.2 g. VI gives 7.5 g. of trimethyl-3-amino-4-hydroxyphenylarsonium chloride (VIA) HCl, m. 211-15°. MeAs(C6H4Br-4)2 (5 g.) and MeI, heated 12 hrs. on the steam bath, give 6 g. of dimethyldi(4-bromophenyl)arsonium iodide, m. 221-4°; the nitrate (VII) m. 195-6°. Nitration of 5 g. VII in 3.5 cc. HNO3 and 8 cc. H2SO4 (heating 15 min. on the steam bath) gives 5.9 g. of dimethyldi(3-nitro-4-bromophenyl)arsonium nitrate, m. 206-7° (decomposition); the bromide m. 183-5° (decomposition); the iodide m. 169-70°. For III the M. T. D. is 30 mg./kg. (rats); the M. L. D. is 40 mg./kg.; at a dosage level of 10 mg./kg. III affords no protection against T. equiperdum infection when administered intravenously. For VIA the M. T. D. is 70-80 mg./kg.; there is no trypanocidal effect at 50 mg./kg. and no germicidal effect was noticed with a 1-100 concentration (pH 2.07) against B. typhosus or Staph. aureus when the pH of the solution is adjusted to 6.75.

IT 756865-34-6P, Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, -HCl
RL: PREP (Preparation)
(preparation of)

RN 756865-34-6 CAPLUS

CN Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, HCl (4CI) (CA INDEX NAME)



● HCl

L24 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1941:35077 CAPLUS

DN 35:35077

OREF 35:5471e-i

TI Synthesis of some iodinated aromatic compounds

AU Long, Louis, Jr.; Burger, Alfred

SO Journal of the American Chemical Society (1941), 63, 1586-9
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

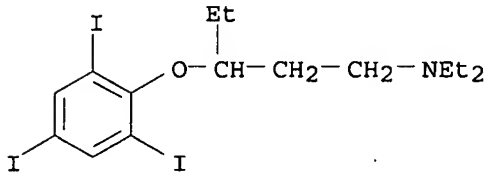
LA Unavailable

AB The following derivs. were prepared for study in clinical x-ray visualization and chemotherapy. 2,4,6-I3C6H2NH2 does not react with AcNHC6H4SO2Cl (I) in C5H5N, C5H5N-Me2CO, PhNMe2 or quinoline; 2,4,6-I3C6H2NHCH2CO2H could not be prepared from HCHO and KCN, ICH2CO2Et or the ester with C5H5N in PhCl; the urea could not be formed from nitrourea in 95% EtOH. Ac2O and concentrated H2SO4 give 2,4,6-triiodoacetanilide, m. 276-7° (decomposition); decomposition occurs with (ClCH2CO)2O. 2,4-I2C6H3NH2 (II) and I in C5H5N, allowed to stand 1 hr. at room temperature and heated 20 hrs. on the steam bath, give 78% of the N4-Ac derivative, m. 230-1°, of N1-2,4-diiodophenylsulfanilamide, pale yellow, m. 176-8° (70% yield on hydrolysis). Addition to a mixture of 1 g. II, 0.3 g. 95% EtOH, 0.01 g. of 30% KOH and 0.12 g. of 40% HCHO at 80° of 0.2 g. boiling 49% aqueous KCN and refluxing for 3 hrs. give 2.1% of 2,4-diiodophenylglycine (III), m. 160-60.5° (decomposition); 1 g. II, 0.62 g. of ICH2CO2Et and 0.23 g. of C5H5N in 13 cc. absolute EtOH, refluxed 17 hrs., give 4.2% of III; PhNHCO2H

(4 g.) in 120 cc. 95% EtOH and 20 cc. concentrated HCl, treated at 0-5° with 6.25 g. KIO3 and 5.86 g. KI in 175 cc. H2O, gives 28% of III. II (6.99 g.) in 125 cc. 95% EtOH and 10 cc. C5H5N, treated with 10.08 g. nitrourea in 4 portions (the reaction mixture being allowed to stand 24 hrs. at room temperature between each addition), gives 29% of 2,4-diiodophenylurea, m. 294-5° (decomposition) after sublimation at 250°/2 mm. Refluxing 7 g. of 2,4,6-I3C6H2OH (IV) and 5 g. ClCH2CO2H with 0.63 g. Na in 60 cc. BuOH for 6 hrs., followed by hydrolysis with 20 cc. of 30% NaOH, gives 74% of 2,4,6-triiodophenoxyacetic acid, m. 224-5° (decomposition); the Na salt may be crystallized from 50 parts of boiling H2O. The Na derivative from 19 g. IV and 7 g. of Et2NCH2CH2Cl in absolute EtOH, refluxed 3 hrs., give 42.6% of the HCl salt, m. 195-6° (decomposition), of 1-diethylamino-2-(2,4,6-triiodophenoxy)ethane, an oil; picrate, yellow, m. 146-8° (decomposition). 1-Diethylamino-3-methyl-3-(2,4,6-triiodophenoxy)propane-HCl, m. 190° (decomposition), 62% yield; the 3-Et homolog m. 188-90° (decomposition). 2,4,6-Triiodophenyl chloroacetate, m. 141-2°.

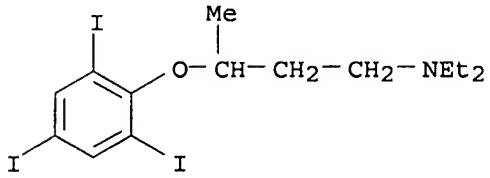
IT 756865-34-6P, Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, -HCl 854391-68-7P, Butylamine, N,N-diethyl-3-(2,4,6-triiodophenoxy)-, -HCl
RL: PREP (Preparation)
(preparation of)

RN 756865-34-6 CAPLUS
CN Amylamine, N,N-diethyl-3-(2,4,6-triiodo-phenoxy)-, HCl (4CI) (CA INDEX NAME)



● HCl

RN 854391-68-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



● HCl